Strategy for the new ferroelectric materials in tetrahedral system

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Recent our summary on the stability diagram of perovskites ABO_3 with octahedral system [Fig.1] has pointed out the importance of chemical bonds of A-O as well as B-O in perovskites[1]. Tolerance factor, which is a useful parameter to consider the structure and the stability of the perovskite, gives an intuitive image of deformation of BO_6 system from cubic (e.g. $SrTiO_3$, $BaZrO_3$) to tetragonal (e.g. $BaTiO_3$, $KNbO_3$, $PbTiO_3$) in the region $t>1$. $GdFeO_3$-type orthorhombic (*Pnma*) distortion is generally known to appear in the region $t<1$ due to the tilting of BO_6. Most important result of Fig.1 is ferroelectric materials appear both in regions $t<1$ and $t>1$. The ferroelectricity of ABO_3 in $t>1$ is intuitively clear from the uniaxially elongated oxygen octahedra. Famous and important ferroelectric materials such as $BiFeO_3$, $BiMnO_3$ (metastable), $BiCoO_3$ (metastable), $PbVO_3$ (metastable), and $CdTiO_3$[2], some of which have larger electric polarization comparable to that of $PbTiO_3$, also exist in the region $t<1$. Chemical bonds between A-O triggers the ferroelectricity in the materials with $t<1$ and the caused polarization is not small compared to the materials in the region $t>1$, as clearly seen in Fig.1. These results encourage us to consider new materials with distorted polyhedra of other coordination numbers, different from perovskites, four[3], five, and seven. Recently we have reported $FeAlO_3$[4] with mixed coordination numbers of 4 and 6. More recently we have just begun the evaluation of the potential of wurtzite system, which was first studied by prof. Sawada's group[5]. Moriwake *et al.*[6] have calculated the possibility of polar materials, including wurtzite materials, switching to ferroelectric by the applied electric field. Detailed calculated data will be presented at the presentation to explore the possibility to get new ferroelectric in the tetrahedral system.

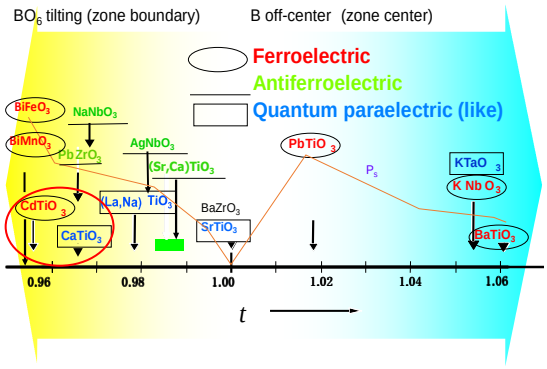

Fig.1 Tolerance factor *t vs.* dielectric/ferroelectric properties of perovskites.

References

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